

Preface

This book aims to bring together continuum elasticity theory, electronic structure and the concept of fractals as applied to roughness and toughness of metals.

Of course, a major contribution to fracture was made by Griffith, in which, though incomplete for reasons that are now largely understood, he derived an expression for the limiting strength of a material. This involved intimately the surface energy, which subsequently, at least in a simple metal like Al with s and p electrons, has been related to the energy of formation of a vacancy. However, a tremendous step forward came with the concept of a dislocation.

It was shown that if a limited area of one plane slips by one atomic distance over the neighbouring plane, the boundary of this area is a closed loop of dislocation. Once this loop is formed, glide can propagate across the plane by the spreading of the area, which is a motion of the dislocation line across its glide plane. General interest in dislocation theory was aroused by its success in providing atomistic theories for plastic deformation and crystal growth. Progress has been made in this field for more than one decade on the treatment of elastic anisotropy and dislocation mobility. For more than two decades, interests have concentrated on deepening our understanding of the structure and role of the dislocation core the behaviour of a pile-up of dislocations (simulating a crack). Interatomic forces (electronic structure) play a decisive role in the structure of the dislocation core and even in fracture. In particular, the temperature dependence of fracture toughness of materials has a close relationship to the interatomic forces. Molecular dynamics has been applied to understand the dislocation motion and the emission of dislocations at the crack tip under loading. Dynamics of crack propagation has become an area of considerable current interest for theoretical physicists and material scientists.

As to electronic structure, electron density theory based on a one-body potential $V(\mathbf{r})$ including electron-electron exchange and correlation interactions has transformed what can be done on electronic structure of both perfect and

defective crystals. Nevertheless, it is still important to subsume ideas involved there into interatomic force fields, which can then be used to study extended defects such as surfaces, grain boundaries, dislocations and cracks. There is still, however, much to do in understanding, in metals, the role of collective effects (including plasmons) in determining mechanical properties and tribology of conducting materials. If our book proves to make a contribution to furthering the progress in relating and enriching ideas from continuum theory, from electronic structure, and from concepts of fractal structure, then that will be more than ample justification for the effort involved in the present project.

We are conscious that in some areas embraced in our book, there is rapid movement at the time of writing. If authors in electron theory or in very practical aspects of materials science and engineering see where we ought to do better, we shall count it a privilege if they write to us with positive suggestions for improvement.

Over a decade or more, diverse scientists have recognized that many of the structures common in their experiments have a special kind of geometrical complexity. Mandelbrot in his pioneering work introduced the concept of fractals and used the idea of a fractal dimension which often is not an integer to characterize the complex structure quantitatively. Fractals may be considered as systems which obey the law of self-similarity, or are self-affine.

Since Mandelbrot *et al.* (1984) showed that fractured surfaces are fractals in nature and that the fractal dimensions of the surfaces correlate well with the toughness of the material, many authors have found that the fractal dimension depends on the fracture properties of materials, but the values of it seem in a narrow range for measurements with a resolution down to the micron scale. This has led to much discussion on the universality and specificity of the fractal dimension of fractured surfaces. However, the roughness index (or local fractal dimension) is found to display wide differences depending on materials on a small length scale by means of scanning electron microscopy (SEM). Another problem is that the negative correlation of the fractal dimension of fractured surfaces with toughness of ductile materials is quite difficult to understand. These basic problems remain open at the time of writing and much remains to be done.

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